A science paradigm shift is needed for Earth and Environmental Systems Sciences (EESS) to integrate Knowledge-Guided Artificial Intelligence (KGAI) and lead new EESS-KGAI theories

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Focal Area

The focal area of this white paper is *learning from complex data through the use of AI techniques and AI-derived model components*. Specifically, we advocate for research programs to develop knowledge-guided AI (KGAI) in the Earth and Environmental Systems sciences (EESS) as a basic research paradigm that is separate from (but supports) any specific Earth system model, modeling components, and modeling workflows, and even separates from specific hypothesis-driven questions about individual Earth system processes.

Science Challenge

Despite long-standing surface hydrology research using process-based approaches, the hydrology community is still unable to formulate scale-relevant theories (Peters-Lidard et al. 2017). Yet artificial intelligence has already been extremely successful at learning inter-catchment process similarities directly from data (Nearing, 2020). Earth and Environmental System Sciences (EESS) has relied on an established process-based approach that follows the integrated Model-Observation-Experiment (ModEx; USDOE 2018) paradigm. We fear however that limiting KGAI to the ModEx science paradigm reduces KGAI to a tool with ad hoc problem-driven solutions to EESS challenges rather than a fundamental scientific method of inquiry. The basic challenge that we see as a transformative geoscience discipline is about how to demystify and embrace AI and combine what we have learned from decades or centuries of scientific progress across the EESS sub-disciplines with the unprecedented ability of KGAI for extracting information directly from observational data.

Our view is that artificial intelligence offers a set of cross-cutting technologies *and* philosophies that can help bridge existing theories of individual processes across spatiotemporal scales. As a transformational EESS vision, we advocate for advancing KGAI technologies in EESS through a paradigm shift toward building EESS-AI theory. Transforming ad hoc progress into more effective guidance is a science problem in its own right, independent of any specific challenge related to predicting the integrated water cycle.

Rationale

There is currently no theory and little guidance for EESS modelers about what types of KGAI strategies exist, how to properly use them, or how to promote the KGAI science contribution to EESS. Attempts to map science contributions between EESS and KGAI sciences (Baker et al., 2019; Reichstein et al., 2019) and promote team building between domain experts, AI experts, and computer scientists are still at their infancy. As a community, we do not currently have a robust and systematic understanding of either (1) the scope of possibilities for integrating EESS process understanding with KGAI, nor (2) optimal strategies for doing so under different classes of modeling problems. KGAI should integrate data driven methods with process-based understanding and predictability into integrated Earth systems models, relying on the best available information from theory and/or data for each component in a complex systems model. KGAI integration should also be explainable, providing a deeper and more generalizable understanding of Earth system

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behavior. This challenge is presently attacked on an ad hoc, case-by-case basis, where different KGAI strategies are applied to different Earth systems hypotheses and prediction problems. Alternatively, we propose to focus on understanding classes of problems where different KGAI strategies work for different reasons.

For example, in a hydrology model, rainfall uncertainty estimation might benefit from a different type of KGAI than watershed scale or hillslope scale surface runoff estimation, which may benefit differently from KGAI than groundwater recharge estimation (which is dominated by landscape and vadose zone heterogeneity), which might itself require different KGAI approaches than groundwater flow problems (which are dominated by parameter uncertainty and preferential flow paths, etc.). Many classes of KGAI strategies will likely be developed for and map well to broad classes of EESS modeling problems. As another example, AI works well for problems of predicting Earth systems of so-called “intermediate complexity”, where mechanistic laws like conservation principles are difficult to apply effectively across heterogeneous environments at relevant scales but where heterogeneity is not great enough to rely on ergodic approximations (Dooge, 1986). The hydrology community has explored the problem of developing scale-relevant theories for systems of intermediate complexity from many different angles with little success (Peters-Lidard et al. 2017), but machine learning has been extremely successful at learning inter-catchment process similarities directly from data (Kratzert et al. 2019). This type of success may or may not translate to classes of problems where mechanistic theories apply well at relevant scales; for example, we would be surprised if AI approaches provided fundamental advantages over Euler approximations of Navier-Stokes solutions for planetary flows (although KGAI likely will provide computational advantages in this area).

The question is: *how can the EESS community build a robust understanding about when, where, and how KGAI integrates well with the many different types of challenges that the EESS community faces*? We propose the need to (i) systematically develop this understanding at a theoretical level involving deep collaboration with the AI/ML and computer science communities, and (ii) for the EESS community to gain a more systematic understanding of the different approaches for KGAI, and how those approaches can be applied to various types of EESS problems. We believe that it is worth developing this type of experience at a basic level, rather than solely through the ad-hoc application of AI strategies to individual EESS grand challenges. In essence, we are proposing that the EESS community (and relevant funding agencies) recognize *hypotheses about EESS-specific KGAI* to be within the purview of the Earth science community, rather than KGAI being a part of traditional EESS hypothesis-driven science.

One of the reasons we believe a paradigm shift is timely and important is because AI conferences like NeurIPS, ICLR, and ICML are becoming as large as any discipline section of Earth science meetings like AGU, EGU, IGARSS, etc. The Earth system community would benefit from efforts dedicated explicitly to building bridges with the AI community, with the goal of helping to lead, rather than chase EESS-relevant AI theory development. We advocate that this perspective could inform funding agencies like DOE, NSF, NASA, NOAA, etc. to (i) develop new research programs that go beyond cross-disciplinary collaboration at the level of technology adoption for solving problems and (ii) take a leadership role in the development of new theory, strategies, and AI practices.

Narrative

To reiterate, the basic long-term challenge that we see is about how to accelerate our ability to combine what the EESS community has learned from decades or centuries of scientific progress across the Earth science sub-disciplines with the unprecedented ability of AI for extracting information directly from observational data. We see this as not only a research problem in its own right within the purview of the EESS community, but also likely as the single greatest challenge for the EESS community in the upcoming decade.

We argue that new science (and culture) paradigms are necessary to achieve this objective, relying on KGAI strategies separate from (but support) ModEx paradigm. The new paradigms need to include sufficient computing resources and innovative software tools (i.e. workflows) for data acquisition, labels and benchmark, and for building and analyzing those KGAI models and approaches that allow for linkages between KGAI and process models / understanding, all in compliance with FAIR principles. As a community however, we still do not currently understand either the scope of possibilities for integrating process understanding with AI, nor the optimal strategies for doing so under different classes of modeling, analysis, hypothesis testing, or prediction problems. KGAI strategies guide the development of the interactions and opportunities between all those elements (data, computing, AI method - i.e. workflow) and scientific contributions. We currently see several classes of emerging strategies for KGAI in Earth System Sciences:

- Adding AI as ad hoc components in existing EESS modeling workflows - e.g., model parameterization (e.g., Chaney, 2016), pre-and post-processing model inputs and outputs (e.g., Frame, 2020), scaling and resolution (e.g., Yuval, 2020; Gauch, 2020), etc.
- Using regularization to constrain AI models with physical principles - e.g., regularized loss functions that penalize deviations from known physical outcomes, training data augmentation.
- Developing architecture constrained deep learning models that enforce physical principles - e.g., monotonicity (e.g., Gupta, 2019; Daw, 2020), conservation (e.g., Beucler, 2019; Hoedt, 2020). This includes strategies like Neural-ODEs (e.g., Lechner, 2020).
- Integrating process relationships as layers in deep learning tensor networks. Tensor-based modeling systems are flexible enough to include any type of modeling component, including explicit biogeophysical relationships (e.g., Jiang, 2020).
- Combining process-based and AI-based models at the level of interacting processes, where different components of the Earth system are represented by different types of models (e.g., Reichstein, 2020).

These broad classes of strategies are descriptive and not comprehensive - based on our current reading of the literature - rather than prescriptive. Deep dives into predictive modeling of the integrated water cycle under extreme conditions, as well as multi-sector dynamics and specifically interactions of human systems as drivers of environmental processes, might be a first step to develop and demonstrate these new paradigms. These two fields have different degrees of maturity in theory and model development, and may lead to different KGAI strategies.

These efforts are critical to developing an understanding of the AI value proposition for EESS research and lead FAIR AI-EESS theories. We envision that with sufficient dedicated effort, within 5-10 years the EESS community could have a more systematic understanding of the different approaches for KGAI, and how those approaches apply to various types of EESS problems.

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